

AMENDMENTS TO THE CLAIMS

This listing of the claims replaces any prior listing of the claims.

1-58 (Canceled)

59. (Withdrawn) A mass spectrometer as claimed in claim 1, further comprising an ion source selected from the group consisting of : (i) an Electrospray (IES) ion source; (ii) an Atmospheric Pressure Chemical Ionisation ("APCI") ion source.; (iii) an Atmospheric Pressure Photo 25 Ionisation ("APPI") ion source; (iv) a Laser Desorption Ionisation ("LDI") ion source; (v) an Inductively Coupled Plasma (ICP) ion source; (vi) an Electron Impact ("EI") ion source; (vii) a Chemical Ionisation ("CI") ion source; (viii) a Field Ionisation ("FI") ion source; (ix) a Fast Atom Bombardment ("FAB") ion source; (x) a Liquid Secondary Ion Mass Spectrometry ("LSIMS") ion source; (xi) an Atmospheric Pressure Ionisation ("API") ion source; (xii) a Field Desorption ("FD") ion source; (xiii) a Matrix Assisted Laser Desorption Ionisation ("MALDI") ion source; and (xiv) a Desorption/Ionisation on Silicon ("DIOS") ion source.

60. (Withdrawn) A mass spectrometer as claimed in claim 1, further comprising a continuous ion source.

61. (Withdrawn) A mass spectrometer as claimed in claim 1, further comprising a pulsed ion source.

62. (Withdrawn) A mass spectrometer as claimed in claim 1, further comprising a mass analyser selected from the group consisting of: (i) a Time of Flight mass analyser; (ii) a quadrupole mass analyser; (iii) a Penning or Fourier Transform Ion Cyclotron Resonance ("FTICR") mass analyser; (iv) a 2D or linear quadrupole ion trap; and (v) a Paul or 3D quadrupole ion trap.

63. (Currently amended) A method of mass spectrometry comprising:

obtaining mass spectral data using a mass spectrometer;

determining a mass to charge ratio of n different species of ion observed in said mass spectral data; and

calculating a respective error band for the determined mass to charge ratio of each of said n different species of ion, wherein calculating comprises estimating a systematic error in the determined mass to charge ratio of each of n different species of ion, and the probability or confidence that the real, true, actual or accepted mass to charge ratio of each of said n different a species of ion falls within its respective calculated error band is greater than or equal to $x\%$, wherein x is ≥ 50 .

64. (Original) A method as claimed in claim 63, wherein n falls within a range selected from the group consisting of: (i) 1; (ii) 2-5; (iii) 5-10; (iv) 10-15; (v) 15-20; (vi) 20-25; (vii) 25-30; (viii) 30-35; (ix) 35-40; (x) 40-45; (xi) 45-50; (xii) ≥ 50 ; (xiii) ≥ 60 ; (xiv) ≥ 70 ; (xv) ≥ 80 ; (xvi) ≥ 90 ; and (xvii) ≥ 100 .

65. (Canceled)

66. (Original) A method as claimed in claim 63, wherein x falls within a range selected from the group consisting of: (i) 50-55; (ii) 55-60; (iii) 60-65; (iv) 65-70; (v) 70-75; (vi) 75-80; (vii) 80-85; and (viii) 85-90.

67. (Original) A method as claimed in claim 63, wherein x falls within a range selected from the group consisting of: (i) 90-91; (ii) 91-92; (iii) 92-93; (iv) 93-94; (v) 94-95; (vi) 95-96; (vii) 96-97; (viii) 97-98; (ix) 98-99; (x) 99-99.5; (xi) 99.5-99.95; (xii) 99.95-99.99; and (xiii) 99.99-100.

68. (Original) A method as claimed in claim 63, further comprising reporting the mass to charge ratio of at least some of said n species of ion together with the respective calculated error band for each mass to charge ratio.

69. (Currently amended) A method as claimed in claim 63, wherein said mass spectral data comprises data relating to ~~the~~ a time that different species of ion were detected.

70. (Original) A method as claimed in claim 69, wherein said data relating to the time that different species of ion were detected is converted into data relating to the mass to charge ratio of said ions.

71. (Original) A method as claimed in claim 70, wherein said data relating to the time that different species of ion were detected is converted into data relating to the mass to charge ratio of said ions by using a calibration function.

72. (Canceled)

73. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the accuracy of a mathematical model used in mass calibration.

74. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to mass calibration.

75. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to using one or more internal references or calibrants.

76. (Currently amended) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises monitoring for changes in ~~the~~ a time of detection of one or more internal references or calibrants.

77. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the stability or instability of said mass spectrometer subsequent to mass calibration.

78. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to drift of said mass spectrometer subsequent to mass calibration.

79. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the effect of changes in the operating conditions of said mass spectrometer subsequent to mass calibration.

80. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the effect of user intervention subsequent to mass calibration.

81. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the effect of external influences on said mass spectrometer subsequent to mass calibration.

82. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the effect of the stability or instability of a power supply of said mass spectrometer subsequent to mass calibration.

83. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the effect of changes in temperature on said mass spectrometer subsequent to mass calibration.

84. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the effect of changes in interference subsequent to mass calibration.

85. (Original) A method as claimed in claim 84, wherein said interference is due to one or more internal reference or calibrant ions interfering with one or more analyte ions.

86. (Original) A method as claimed in claim 84, wherein said interference is due to one or more analyte ions interfering with one or more internal reference or calibrant ions.

87. (Original) A method as claimed in claim 84, wherein said interference is due to one or more background or chemical noise ions interfering with one or more internal reference or calibrant ions.

88. (Original) A method as claimed in claim 84, wherein said interference is due to one or more background or chemical noise ions interfering with one or more analyte ions.

89. (Currently amended) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating ~~the~~ a time elapsed since said mass spectrometer was last calibrated.

90. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the effect of thermal expansion of one or more components of said mass spectrometer subsequent to mass calibration.

91. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to space charge repulsion effects within said mass spectrometer.

92. (Original) A method as claimed in claim 63, wherein the error due to space charge repulsion effects is determined at least in part by consideration of the observed intensity of one or more species of ions.

93. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error recorded during mass calibration.

94. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the statistical error or random error in determining the mass to charge ratio of said ions.

95. (Currently amended) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the uncertainty or standard deviation of ~~the~~ a time of detection of one or more species of ion.

96. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the uncertainty or standard deviation of the frequency of detection of one or more species of ion.

97. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to ion detection statistics.

98. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to insufficient sampling.

99. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to computational errors.

100. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to rounding off errors.

101. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error in a report exception situation wherein one or more species of ion within said mass spectral data are sufficiently corrupted or suffering from interference that the calculated respective error band of said ions is not reported.

102. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to mass interference wherein background or interference ions having substantially similar mass to charge ratios to analyte ions affect the ability of resolving the analyte ions from said background or interference ions.

103. (Original) A method as claimed in claim 102, wherein the error due to mass interference is estimated by comparing the shape of an observed mass peak from said mass spectral data with the shape of a theoretical mass peak.

104. (Original) A method as claimed in claim 102, wherein the error due to mass interference is estimated by comparing the deviation of the shape of an observed mass peak with either a

Gaussian distribution, a cosine squared distribution, another mathematical function, or a profile derived from the shape of one or more mass peaks of one or more internal reference or calibrant ions.

105. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to saturation of a detector.

106. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to signal amplification saturation.

107. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to deadtime effects or missed counts of an ion counting detector.

108. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to the response of an ion detector.

109. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises estimating the error due to the response of an electron or photon multiplier.

110. (Original) A method as claimed in claim 63, wherein the step of calculating a respective error band comprises combining multiple estimates of different errors.

111. (Original) A method as claimed in claim 110, wherein said multiple estimates of different errors are added in quadrature.

112. (Original) A method as claimed in claim 63, further comprising searching a database to look for one or more ions known to have mass to charge ratios within a range which is related to the determined mass to charge ratio of one or more ions and the respective calculated error band for the determined mass to charge ratio.

113. (Original) A method as claimed in claim 112, wherein said database comprises details of biopolymers, proteins, peptides, polypeptides, oligonucleotides, oligonucleosides, amino acids, carbohydrates, sugars, lipids, fatty acids, vitamins, hormones, portions or fragments of DNA, portions or fragments of cDNA, portions or fragments of RNA, portions or fragments of mRNA, portions or fragments of tRNA, polyclonal antibodies, monoclonal antibodies, ribonucleases, enzymes, metabolites, polysaccharides, phosphorolated peptides, phosphorolated proteins, glycopeptides, glycoproteins or steroids.

114. (Original) A method as claimed in claim 112, wherein said database comprises details of the Electron Impact mass spectra of compounds.

115. (Original) A method as claimed in claim 63, further comprising calculating elemental compositions having mass to charge ratios within a calculated error band of the determined mass to charge ratio of one or more species of ion.

116. (Original) A method as claimed in claim 115, wherein said elemental compositions are calculated using the known masses or mass to charge ratios of atomic elements or groups of elements and/or their isotopes.

117. (Original) A method as claimed in claim 63, further comprising:

defining one or more compounds of interest; and

interrogating at least some of the determined mass to charge ratios and respective calculated error bands of at least some of said different species of ion observed in said mass spectral data to see whether said one or more compounds of interest fall within the error band of at least some of said different species of ion.

118. (Original) A method as claimed in claim 63, further comprising:

defining one or more mass to charge ratios of interest; and

interrogating at least some of the determined mass to charge ratios and respective calculated error bands of at least some of said different species of ion observed in said mass

spectral data to see whether said one or more mass to charge ratios of interest fall within the error band of at least some of said different species of ion.

119. (Original) A method as claimed in claim 63, further comprising:

defining one or more compounds of interest; and

interrogating at least some of the determined mass to charge ratios and respective calculated error bands of different species of ion observed from a plurality of mass spectra acquired over a period of time to see whether said one or more compounds of interest fall within the error band of at least some of said different species of ion observed from said plurality of mass spectra.

120. (Original) A method as claimed in claim 63, further comprising:

defining one or more mass to charge ratios of interest; and

interrogating at least some of the determined mass to charge ratios and respective calculated error bands of different species of ion observed from a plurality of mass spectra acquired over a period of time to see whether said one or more mass to charge ratios of interest fall within the error band of at least some of said different species of ion observed from said plurality of mass spectra.

121. (Withdrawn) A mass spectrometer as claimed in claim 63, further comprising an ion source selected from the group consisting of: (i) an Electrospray ("ESI") ion source; (ii) an Atmospheric Pressure Chemical Ionisation ("APCI") ion source; (iii) an Atmospheric Pressure Photo Ionisation ("APPI") ion source; (iv) a Laser Desorption Ionisation ("LDI") ion source; (v) an Inductively Coupled Plasma ("ICP") ion source; (vi) an Electron Impact ("EI") ion source; (vii) a Chemical Ionisation ("CI") ion source; (viii) a Field Ionisation ("FI") ion source; (ix) a Fast Atom Bombardment ("FAB") ion source; (x) a Liquid Secondary Ion Mass Spectrometry ("LSIMS") ion source; (xi) an Atmospheric Pressure Ionisation ("API") ion source; (xii) a Field Desorption ("FD") ion source; (xiii) a Matrix Assisted Laser Desorption Ionisation ("MALDI") ion source; and (xiv) a Desorption/Ionisation on Silicon ("DIOS") ion source.

122. (Withdrawn) A mass spectrometer as claimed in claim 63, further comprising a continuous ion source.

123. (Withdrawn) A mass spectrometer as claimed in claim 63, further comprising a pulsed ion source.

124. (Withdrawn) A mass spectrometer as claimed in claim 63, further comprising a mass analyser selected from the group consisting of: (i) a Time of Flight mass analyser; (ii) a quadrupole mass analyser; (iii) a Penning or Fourier Transform Ion Cyclotron Resonance ("FTICR") mass analyser; (iv) a 2D or linear quadrupole ion trap; and (v) a Paul or 3D quadrupole ion trap.